CONFORMATIONAL LANDSCAPE OF 3-METHOXYPHENOL INVESTIGATED BY JET-COOLED HIGH RESOLUTION INFRARED SPECTROSCOPY

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Methoxyphenol (MP) are biogenic volatile organic compounds which contribute significantly to biomass burning emissions. MP compounds are able to chemically evolve in the atmosphere and several studies aimed to determine the kinetics and the reactivity intermediates involved in the tropospheric oxidation processes and the subsequent production of secondary organic aerosols whose impact to the climate seems to be decisive.[1] The gas phase monitoring of MP in the atmosphere requires precise rovibrational cross-sections measurements which can be accurately simulated only if the rotational structures both in the vibrational ground state (GS) and excited states (ES) are understood. Recent rotational studies reported about ortho (2-MP), meta (3-MP) and para (4-MP) isomers enabled to characterize their conformational landcape from GS rotational and quartic centrifugal constants to reproduce the millimeter-wave spectra at the experimental accuracy.[2,3] Any vibrational spectrum of MP compounds resolved in rotation could not be recorded so far, mainly due both to the presence of hot bands and to the complexity of the conformational landscape. Taking advantage of our tunable quantum cascade laser spectrometer coupled to a pulsed slit jet [4] we recorded the infrared spectrum of the ν_{18} ring in plane bending mode of the 3-MP isomer around 950 cm^{-1}. Rovibrational analyses supported by the full characterization of the conformational landscape in the GS state [2] provide for the first time unambiguous infrared signatures of two out of four possible conformers of 3-MP including a reliable set of ES rotational constants. A more extensive study in the region of CC ring stretching modes is currently in progress to resolve the four conformational signatures of 3-MP and to bring new insights about the conformational flexibility of these compounds.

References : [1] A. Lauraguais et al. Atm. Envir. 86, 155-163 (2014).[2] A. Roucou et al. CPC 19, 1-8 (2018). [3] A. Jabri et al., accepted in JCP (2019). [4] P. Asselin et al. PCCP 19, 17224-17232 (2017).